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The infra-red bands of strontium oxide

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With 4 figures in the text

Abstract

A band-system of strontium oxide situated in the infra-red part of the spectrum has been investigated. The analysis shows that the system is a $^1\Sigma - {}^1\Sigma$ transition.

The following 7 bands have been analysed: 4,1, 3,0, 3,1, 2,0, 1,0, 0,0 and 0,1. In the upper vibrational levels several perturbations were found. Some of the perturbations are rather considerable and they displace the positions of the heads and the origins. The band-constants derived are as follows:

$$B_v' = 0.3047_1 - 0.0011_2\,(v + \tfrac{1}{2})\ \text{cm}^{-1}; \qquad B_v'' = 0.3377_9 - 0.0020_4\,(v + \tfrac{1}{2})\ \text{cm}^{-1}$$

$$D_v' = 0.32 \cdot 10^{-8} \qquad D_v'' = [0.34_2 + 0.02_4\,(v + \tfrac{1}{2})] \cdot 10^{-8}$$

$$r_e' = 2.027 \cdot 10^{-8}\ \text{cm} \qquad r_e'' = 1.923 \cdot 10^{-8}\ \text{cm}$$

$$\omega_e' \sim 624\ \text{cm}^{-1} \qquad \omega_e'' = 653.4_9\ \text{cm}^{-1}$$

$$x_e' \omega_e' \sim 2 \qquad x_e'' \omega_e'' = 4.0_0$$

Introduction

The introduction of strontium salts in a flame or in the carbon arc gives a complicated band-spectrum, attributed to strontium oxide, stretching from the ultra-violet far into the infra-red part of the spectrum. MECKE and GUILLERY (1) made an attempt to collect some blue bands into a head-equation. They obtained the following result

$$\nu_h = 24638 + 516\,n' - 3\,n'^2 - 648\,n'' + 3.9\,n''^2.$$

Some years later MAHANTI (2) gave a similar head-equation for the blue bands and, in addition, a head-equation for some ultra-violet bands. He got for the blue bands

$$\nu_h = 24702.81 + 519.09\,(v' + \tfrac{1}{2}) - 3.50\,(v' + \tfrac{1}{2})^2 - 653.47\,(v'' + \tfrac{1}{2}) + 4.02\,(v'' + \tfrac{1}{2})^2,$$

and for the ultra-violet ones

$$\nu_h = 28622.18 + 497.81\,(v' + \tfrac{1}{2}) - 5.97\,(v' + \tfrac{1}{2})^2 - 679.13\,(v'' + \tfrac{1}{2}) + 9.13\,(v'' + \tfrac{1}{2})^2.$$

The analyses for the blue bands made by MECKE and GUILLERY and MAHANTI agree very well. In the red part of the spectrum QUERBACH (3) found five red-shaded bands at λ 7860, 7882, 7905, 8257 and 8700 Å. MAHLA (4) made head-measurements of several infra-red bands and reported both a vibrational and rotational analysis. He analysed rotationally the bands at 8257, 8700, 7882 and 7853 Å. He considered them to be the 0,2, 0,3, 3,4 and 0,1 transitions of a $^1\Sigma - {}^1\Sigma$ system. He gave the following head-equation

$$\nu_h = 13358.16 + 628.45\,(v' + \tfrac{1}{2}) - 6.25\,(v' + \tfrac{1}{2})^2 - 633.14\,(v'' + \tfrac{1}{2}) + 2.35\,(v'' + \tfrac{1}{2})^2.$$

His analysis shows no levels in common with those of the blue and ultra-violet systems. He found $B_e' = 0.3373$ and $B_e'' = 0.3738$ cm^{-1}, corresponding to the nuclear distances $r' = 1.92$ and $r'' = 1.82 \cdot 10^{-8}$ cm. He found some perturbations in the lower vibrational levels, the upper ones he considered unperturbed. A peculiarity mentioned by MAHLA is the irregular intensity distribution of the bands, particularly those belonging to the $\Delta v = -1$ sequence. The first two bands are very weak, the subsequent ones more intense.

MEGGERS (5) discovered new bands in the infra-red situated at λ 9196, 9776, 10426 and 10437 Å. He did not, however, give any head-equation.

In plates of the band-spectrum of strontium oxide between λ 7500 and λ 11000 Å, we observe seven marked sequences. At shorter wavelengths the appearance of the spectrum becomes more and more complicated indicating several band-systems. At about 7000 Å the spectrum is completely chaotic. The simplest way to arrange these seven sequences into a vibrational array is to fix the greatest frequency-distance between two consecutive sequences. This occurs between the 9196 and 9776 bands, where the distance between the heads are 645.36 cm^{-1}. Thus we assumed that the 9196 band is the 0,0, the 9776 band the 0,1 transition. This distance agrees surprisingly well with $\Delta G(\frac{1}{2})$ for the lower level of the blue bands. With Mahanti's values we obtain 645.43 cm^{-1}. With the assumption that the 9196 band is the 0,0 transition, it is possibly to arrange most of the bands into a vibrational scheme. The heads are collected in Table 1. Rotational analyses were carried out of 7 bands, namely the 4,1, 3,0, 3,1, 2,0, 1,0, 0,0 and 0,1 transition. MAHLA made rotational analyses of four bands namely our 4,1, 3,0, 2,0 and 1,0 bands, which he considered to 3,4, 0,1, 0,2 and 0,3 transitions. The perturbed levels are the upper ones, not the lower ones as stated by MAHLA. MAHLA's analysis is correct in most places but for the J-numbering. Thus the J-numbering of his R-branch must be decreased by one unit and that of his P-branch increased by one.

MAHLA published tables containing his head-measurements. Several of his bands we cannot find on our plates, some of them seem to us to be non-existent.

Table 1

The band-heads of the infra-red system. The head are given in cm^{-1} and in brackets in Å

6			13256.13 cm^{-1} (7541.60 Å) 604.52	
5		13289.22 637.61 (7522.83) 606,02	12651.61 (7901.96)	
4	13328.55 645.35 (7500.63) 597.80	12683.20 (7882.28) 597.80		
3	12730.75 645.35 (7852.84) 624.33	12085.40 (8272.18) 623.82		
2	12106.42 644.84 (8257.82) 615.35	11461.58 638.29 (8722.5)	10823.29 (9236.80)	
1	11491.07 (8700.02) 619.54			9578.6 (10437.1)
0	10871.53 645.35 (9195.82)	10226.18 637.58 (9776.15)	9588.6 (10426.2)	
↑ v' / v'' →	0	1	2	3

Experimental

Spectrograms were taken in both the first and second order of a plane grating (with a dispersion of 4.5 and 10 Å/mm respectively) and in the first order of a Wood's 21 ft concave grating (with a dispersion varying from 0.95 to 1.15 Å/mm in the region in question). As source of light we used an arc burning in air between carbon electrodes, the upper negative, the lower positive. The current was 5—10 amp. taken from a 440 volts D. C. output. The lower electrode was a carbon cylinder filled with fused strontium chloride. The carbon cylinder was filled with salt while a big alternating current of about 200 amp. was led through the cylinder. The method was employed by BRODERSEN (6). When burning in oxygen atmosphere, the intensity of the strontium bands from the light source did not increase very much. We therefore, preferred to use an arc burning in air. The plates used were Eastman Kodak IL, IM, IN and IZ, which were hypersensitised with ammonia before exposure.

In the concave grating the spectrum was photographed from λ 7000 to 10100 Å. The exposure time varied from 7 to 15 hours. In the plane grating plates were taken of the spectrum from 7000 Å to 11000 Å. Above 10300 Å spectrograms were taken in the first order of the plane grating. The exposure time varied from 1 to 4 hours. For comparison, iron lines were used for the concave grating exposures, and barium, chromium, iron and strontium lines for those with the plane grating.

Description of the bands

As Table 1 shows, the bands form an open Condon parabola. In the sequence $\Delta v = -2$, the 1,3 band is a little more intense than the 0,2. The 0,1, 0,0, 1,0 and 2,0 bands are very intense. The 3,1 band is not so strong as 2,0. The 3,0 and 4,1 bands are of about the same intensity, 4,1 perhaps stronger, 5,1 is stronger than 4,0. A peculiarity is that in the sequence $\Delta v = 0$ it is possible to discover an extremely weak 2,2 band at 10823. 29 cm^{-1} but not the 1,1 band. The 2,1 band is very weak.

Figs. 1 and 2 show the appearance of some of the bands, which are red-shaded. Every band consists of two branches, one R and one P-branch indicating a $^1\Sigma - {}^1\Sigma$ transition. Table 1 gives the head-measurements and shows that the levels $v' = 3$ and 4 of the upper state are displaced. This depends on interactions between the upper state and unknown electronic states.

The analysis is complicated by the existence of several perturbations in the bands. Some of them are extremely large, especially that in the level $v' = 0$ at $J = 36$, 37 (See Fig. 2 and 4). Another large perturbation occurs in the beginning of the level $v' = 3$ and causes a considerable displacement of the heads of the 3,0 and 3,1 bands. The head of the 4,1 band is also displaced due to a perturbation.

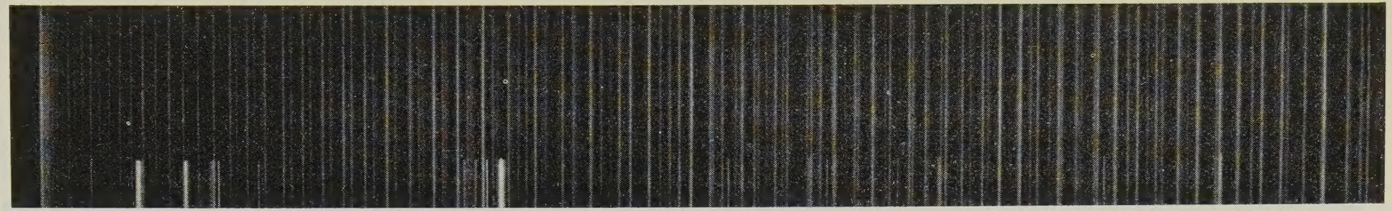
The wave-numbers of the band-lines are given in Tables 2—3. Overlapped, blended or unresolved lines are marked with an asterisk *. All the band-lines measured are from plates taken with the concave grating. Generally the errors in measurements do not exceed $\pm$ 0.03 cm^{-1}. The wavelengths of the atomic lines used for comparison are taken from the M. I. T. list (7). In order to indicate the validity and accuracy of the analyses, the combination differences of the lower levels $v'' = 0$ and $v'' = 1$ are given in Tables 4—5.

Strontium has four isotopes with atomic weights 84, 86, 87 and 88 and with a relative abundance of 0.6 : 9.8 : 7.0 : 82.7. The plates show several weak lines that might be referred to the less abundant isotopes. We have, however, not made any effort to obtain other lines than those belonging to the most abundant isotope.

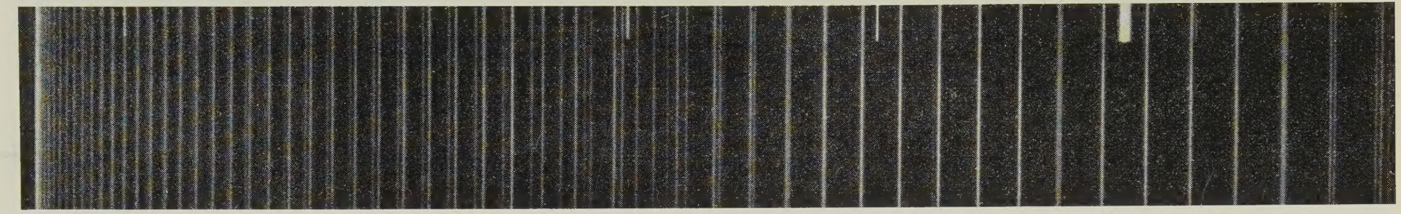
Analysis

Rotational analysis

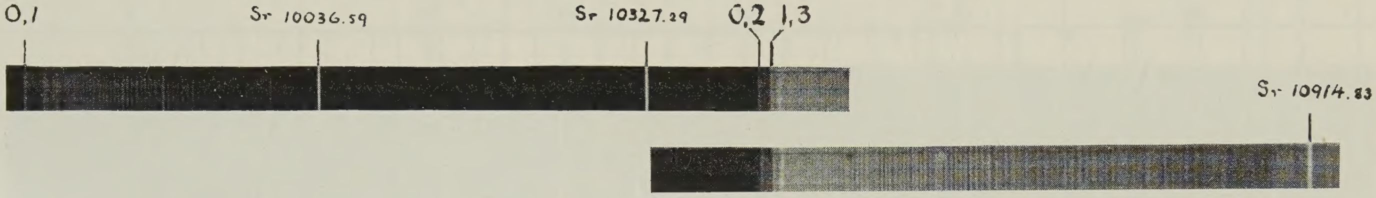
Rotational analyses are made of 7 bands, four of them with lower level $v'' = 0$, namely 3,0, 2,0, 1,0 and 0,0 and the other three with lower level $v'' = 1$, namely 4,1, 3,1 and 0,1. All the bands are perturbed. The 2,0 and



The 2,0 band at 8258 Å

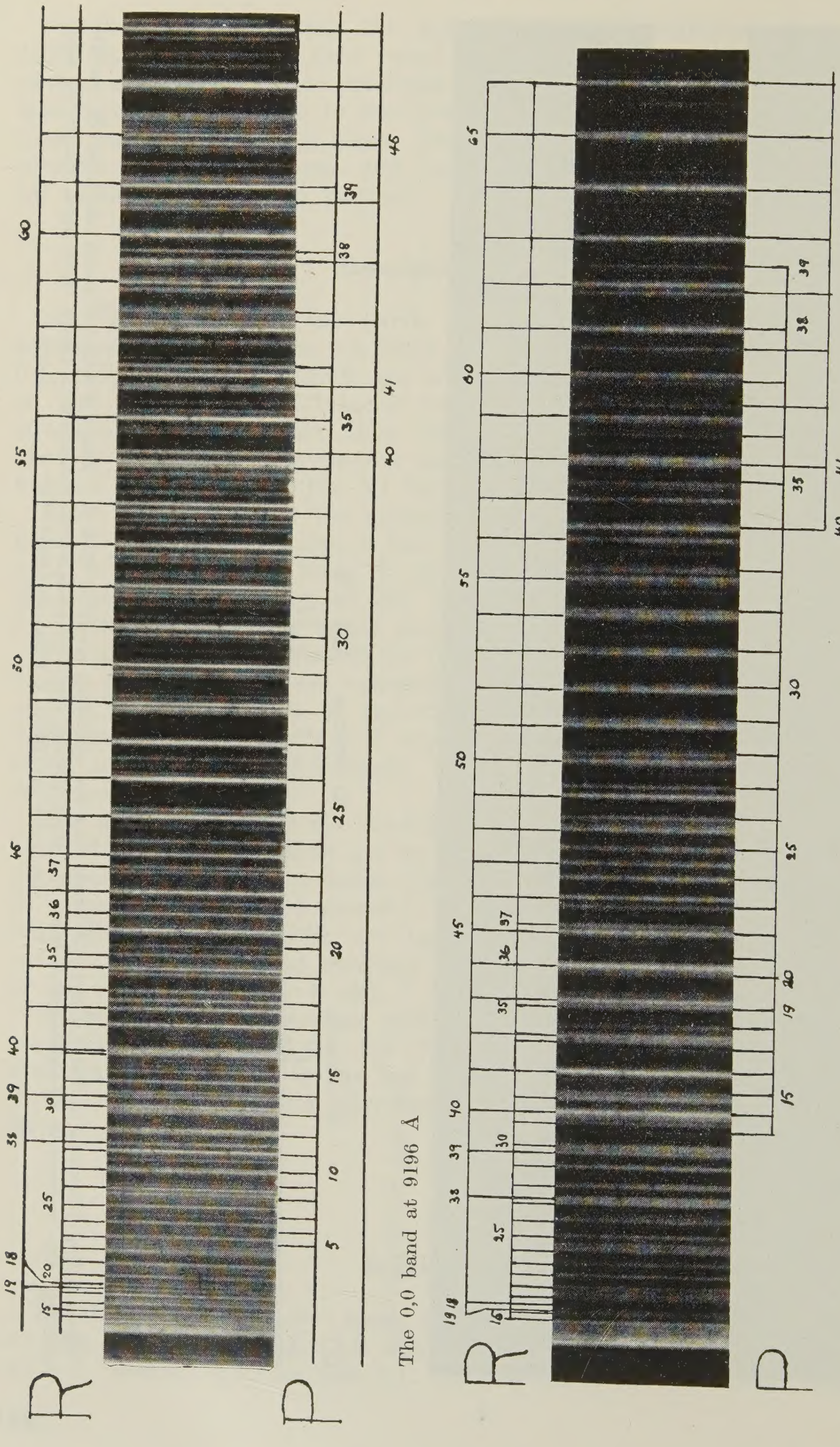


The 1,0 band at 8700 Å



The 0,1, 0,2 and 1,3 bands at 9776, 10426 and 10437 Å

Fig. 1. Reproductions of the 2,0 and 1,0 bands and the spectrum above λ 9750 Å. The 2,0 and 1,0 bands are from the concave grating, the undermost reproduction is from the plane-grating (for this part of the spectrum IZ-plates were used, which are more sensitive at 10400 Å than at 10000 Å).



The 0,0 band at 9196 Å

The 0.1 band at 9776 Å

Fig. 2. Reproductions of the 0,0 and 0,1 bands showing the R and P-branches with perturbations at $J = 19.5$ and 38.5.

Table 2

Wave-numbers for the 0,0, 0,1 and 1,0 bands

J	0,0		0,1		1,0	
	$R(J)$	$P(J)$	$R(J)$	$P(J)$	$R(J)$	$P(J)$
1	10869.65					
2	70,02					
3	70.39	10866.21*				
4	70.77*	65.42				
5	71.11*	64.51				
6	71.32*	63.49				11483.05
7	71.53*	62.42				82.04
8	71.53*	61.23	10226.17*	10215.93		80.84
9	71.53*	60.06	26.17*	14.66		79.58
10	71.53*	58.78	26.17*	13.50		78.29
11	71.32*	57.41*	26.17*	12.15*		76.95
12	71.11*	55.96	25.88	10.72		75.52
13	70.77*	54.44	10225.65	09.26	11490.38	74.02
14	70.39*	52.88	25.34	07.93*	90.04	72.47
15	69.91	51,25	24.95	06.28	89.62	70.85
16	69.38	49.52	24.49	04.61*	89.12	69.19
17	68.67	47.67*	23.84	02.85	88.57	67.41
18	67.84	45.81	23.06	01.13	87.95	65.59
19	68.24	43.78	23.49	10199.01*	87.27	63.67
20	67.19	41.55	22.64	96.91	86.50	61.73
21	66.21*	40.77	21.66	96.21*	85.66	59.68
22	65.16	38.27	20.78	93.88	84.81	57.58
23	64.11	35.91	19.76	91.53	83.84	55.40
24	62.95	33.55	18.72	89.35	82.81	53.17
25	61.71	31.14	17.58	87.01	81.71	50.89
26	60.38	28.62	16.40	84.54	80.56	48.50
27	58.97	25.93*	15.10	82.15	79.31	46.07
28	57.41*	23.37	13.68	79.63	78.02	43.55
29	55.75	20.63	12.15*	77.00	76.66	40.99
30	53.98	17.75	10.52	74.25	75.22	38.35
31	52.04	14.77	08.70	71.42	73.72	35.66
32	49.96	11.64	06.78	68.45	72.15	32.87
33	47.67*	08.36	04.61*	65.35	70.50	30.01
34	45.10	04.92	02.21	61.97	68.79	27.14
35	42.27	01.33*	10199.49	58.50	67.03	24.13
36	39.06	10797.39	96.23*	54.72	65.18	21.13*
37	35.56	93.25	93.12	50.83	63.24	17.98*
38	56.85	88.73	10214.50	46.19	61.25	14.78*
39	53.18	83.85*	11.11	41.81	59.18	11.48*
40	49.74	10803.86	07.83*	61.97	57.02	08.16
41	46.49	10798.83	04.61*	57.10	54.78	04.82*
42	43.38	94.03	01.80	52.53	52.46	01.32*
43	40.37	89.44	10199.01*	47.99	49.99	11397.78*
44	37.43	84.99	96.47	43.85	47.31	94.13*
45	34.56	80.67	93.56	39.64*	44.21	90.25
46	31.67	76.40	90.90	35.84	46.56	86.28
47	28.90	72.15*	88.23	31.62	42.36	81.85
48	25.93*	67.95*	85.57	27.68*	39.10	82.90
49	23.03	63.79	82.90	23.58	36.03	77.32
50	20.07	59.58	80.14	19.66	33.30	72.74

Table 2. (Cont.).

J	0,0		0,1		1,0	
	$R(J)$	$P(J)$	$R(J)$	$P(J)$	$R(J)$	$P(J)$
51	17.10	55.34	77.39	15.66*	30.25	68.42
52	14.04	51.09	74.63	11.58	27.25	64.17
53	10.95	46.78	71.77	07.53	24.26	59.90
54	07.84	42.41	68.86	03.41	21.13*	55.60
55	04.61	38.00*	65.89	10099.25	17.98*	51.27
56	01.33*	33.57	62.90	95.02*	14.78*	46.87
57	10798.01	29.04	59.78	90.73	11.48*	42.39
58	94.62	24.46	56.67	86.42	08.40	37.86
59	91.13	19.76	53.47	81.99	04.82*	33.22
60	87.56	15.04	50.05	77.58	01.32*	28.86
61	83.86*	10.25	46.72	73.03	11397.78*	23.97
62	80.10	05.34	43.08	63.38	94.13*	19.16
63	76.17	00.37	39.64*	63.68	90.44	14.31
64	72.15*	10695.27	35.69	58.88	86.66	09.34
65	67.95*	90.06	31.89	54.10	82.48	04.28
66	63.49	84.69	27.68*	48.96	77.68*	11299.13
67	58.76	79.16	23.29	43.71	77.68*	93.73
68	53.60	73.42	18.44	38.31	72.57	87.56
69	47.91	67.37	13.06	32.57	68.14	86.34
70	41.40	60.93	06.84	26.39	63.81	79.86
71	63.48	53.92	29.26	19.70	59.49	74.17*
72	56.13	46.08	22.17	12.21	55.12	68.53*
73	49.50	66.90	15.76*	33.34	50.62	62.86
74	43.47	58.25	10.28	25.03	46.04	57.28*
75	38.00*	50.39	05.01	17.40	41.26	51.45*
76	32.47	42.98	10099.87	10.41	36.08	45.54
77	27.16	36.04	95.02*	03.88	30.00	39.49
78	21.68	29.36			34.45	33.06
79	16.37	22.75			27.36	25.73
80		15.99			21.43	28.84

J	1,0		J	1,0		J	1,0	
	$R(J)$	$P(J)$		$R(J)$	$P(J)$		$R(J)$	$P(J)$
81	11316.13	11220.38	96	32.22	19.33	111	44.94	14.59
82	10.97	13.31	97	24.50	11.71	112	37.11	05.91
83	05.83	06.72	98	16.16	03.60	113	30.23	10997.49
84	00.70	00.25	99	27.64	11094.65	114	21.84	89.08
85	11295.51	11193.84	100	18.60	84.90	115	22.54	80.32
86	90.28	87.39	101	10.52	95.19	116	12.86	70.65
87	84.99	80.91	102	04.08	84.90	117	04.90	70.16
88	79.61	74.40	103	11197.11	75.55	118	11097.32	59.26
89	74.17*	67.84	104	90.33	67.85	119	89.59	50.07
90	68.63*	61.20	105	83.50	59.64	120	82.47	41.24
91	62.98	54.51	106	76.44	51.63	121	74.87	32.30
92	57.28*	47.70	107	68.50*	43.51	122	67.20	23.98
93	51.45*	40.80	108	68.50*	35.19	123	59.37	15.15
94	45.37	33.79	109	59.57	26.01			
95	39.19	26.66	110	52.13	24.83			

Table 3

Wave-numbers for the 2,0, 3,0, 3,1 and 4,1 bands

J	2,0		3,0		3,1		4,1	
	R(*J*)	*P*(*J*)	*R*(*J*)	*P*(*J*)	*R*(*J*)	*P*(*J*)	*R*(*J*)	*P*(*J*)
3		12101.25						
4		00.41						
5		12099.50						
6		98.44						
7		97.39						
8		96.23						
9		—						
10		93.67						
11		92.33						
12	12105.95	90.89						
13	05.65	89.38			12076.66		12682.28	
14	05.31	87.78	12721.22		76.13		12681.84*	
15	04.86	86.13	20.42		75.34	12057.23*	81.38	12662.87*
16	04.36	84.42	19.55	12700.29	74.52	55.32	80.80	61.11
17	03.78	82.65	18.65	12698.20	73.74	53.17*	80.12	59.31
18	03.14	80.80	17.68	95.98	72.92	51.17	79.51	57.42
19	02.43	78.90	16.72	93.73	72.00	48.99	78.80	55.47*
20	01.64	76.87	15.69	91.45	71.06	46.70*	77.92	53.46
21	00.75	74.83	14.65	89.12*	70.07	44.61*	77.01	51.34
22	12099.85	72.69	13.50	86.77	69.07*	42.30	75.96	49.17*
23	98.84	70.49	12.31	84.27	67.92	39.87*	74.86	46.86
24	97.78	68.24	11.08	81.84*	66.77*	37.59	73.63	44.55
25	96.67	65.88	09.77	79.29	65.57	35.18	72.25	42.10
26	95.45	63.45	08.36	76.71	64.38*	32.71	70.65	39.54
27	94.18	60.98	06.94	74.07	63.05	30.20	68.64*	36.86
28	92.85	58.45	05.47	71.39	61.67	27.55*	72.93	33.88*
29	91.44	55.85	03.93	68.64*	60.26	24.99	70.42	30.59*
30	89.96	53.17*	02.32	65.78	58.79	22.28	68.18	33.59
31	88.40	50.41	00.59	62.87*	57.23*	19.52	66.11	29.67
32	86.77	47.59	12698.85	59.95	55.64	16.71	64.36*	26.08
33	85.08	44.71*	97.10	56.94	53.96	13.81	62.45	22.74
34	83.33	41.76	95.19	53.80	52.28	10.91	60.52	19.53
35	81.49	38.71	93.22	50.70	50.40	07.89	58.56*	16.35
36	79.61	35.63	91.21	47.46	48.65*	04.86	56.62	13.13
37	77.63	32.46	89.12*	44.14	46.70*	01.71	54.57	09.84
38	75.61	29.22	86.92	40.81	44.61*	11998.52	52.42	06.52
39	73.49	25.95	84.70	37.34	42.59	95.28	50.33	03.18
40	71.34	22.57	82.44	33.88*	40.49	91.94	48.12	12599.85*
41	69.07*	19.11	80.12	30.33	38.30	88.58	45.87	96.27*
42	66.77*	15.59*	77.60	26.66	36.04	85.12*	43.47	92.78
43	64.38*	12.04	75.13	23.03*	33.71	81.66*	41.05	89.15
44	61.96	08.39	72.53	19.23	31.37	78.06	38.55	85.49
45	59.43	04.68	69.85	15.41	28.90	74.40	35.97	81.72
46	56.85	00.90	67.15	11.46	26.35	70.72	33.28	77.91
47	54.20	11997.07*	64.36*	07.50	23.76	66.94	30.59*	74.00
48	51.45	93.14	61.47	03.43*	21.11	63.08	27.75*	70.02
99	48.65*	89.15	58.56*	12599.32	18.38	59.12*	24.68*	65.97
50	45.82	85.12*	55.47*	95.10	15.59*	55.18	24.31	61.77
51	42.89	81.00	52.42	90.85	12.69	51.17	20.32	57.44
52	39.87*	76.81*	49.17*	86.49	09.73	47.03	16.74	55.79

Table 3. (Cont.).

J	2,0		3,0		3,1		4,1	
	$R(J)$	$P(J)$	$R(J)$	$P(J)$	$R(J)$	$P(J)$	$R(J)$	$P(J)$
53	36.72	72.55	45.87	82.08	06.68	42.84	13.48*	50.44
54	33.35	68.23	42.51	77.55	03.51	38.59*	10.19	45.57
55	31.14	63.78	39.00	72.91	00.29	34.20	06.83	40.97
56	27.55*	59.12*	35.43	68.24	11997.07*	29.76	03.43*	36.37
57	24.12	55.48	31.56	63.40	93.36	25.22	12599.85*	31.69
58	20.69	50.60	27.75*	58.44	89.79	20.52	99.27*	27.03
59	17.19	45.87	23.03*	53.32	85.39	15.63	92.48	22.24
60	13.64	41.12	17.54	48.22	80.20	10.81	88.48	17.31
61	10.05	36.33	24.65*	42.18	87.45	04.99	84.04	12.16
62	06.36	31.46	18.52	35.39	81.66*	11898.57		06.86
63	02.62	26.56	13.48*	41.04	77.02	11904.51		01.08
64	11998.83	21.59	09.03	33.78	72.75	11897.49		
65	94.97	16.51	04.66	27.47	68.62	91.45		
66	91.02	11.40	00.32	21.62	64.58	85.88		
67	87.02	06.22	12595.97	15.90	60.55	80.46		
68	82.96	00.97	91.66	10.32	56.45	75.11		
69	78.83	11895.66	87.22	04.63	52.37	69.78		
70	74.64	90.28	82.76	12498.93	48.26	64.42		
71	70.37	84.84	78.27	93.22	44.06	59.03		
72	66.02	79.33	73.65	87.48	39.81	53.60		
73	61.63	73.74	68.95	81.59	35.42	48.12		
74	57.17	68.14	—	75.44	30.35	42.43		
75	52.62	62.44	59.42	69.76	27.09	36.80		
76	48.02	56.67	54.98	63.88	22.51	30.54		
77	43.34	50.83		57.56	17.93	25.99		
78	38.59*	44.93		51.92	13.30	20.11		
79	33.80	38.96			08.58	14.25		
80	28.86	32.94			03.79	08.32		
81	23.62	26.82			11898.68	02.33		
82		20.60			93.72	11796.27		
83						90.10		
84						83.67		

1,0 bands are the easiest ones to analyse. As Table 2 shows, we were able to follow the branches of the 0,1 band to such a high J-value as $J = 123$, $R(123)$ and $P(123)$. The stumbling-block in the whole analysis was the large perturbation in the upper level $v' = 0$. Fig. 2 shows this remarkable perturbation in both the 0,0 and 0,1 bands.

The band-constants for the unperturbed lower levels $v'' = 0$ and $v'' = 1$ are determined by the usual graphical method, plotting $\Delta_2 F''(J)/(J + \frac{1}{2})$ against $(J + \frac{1}{2})^{\frac{1}{2}}$. The dots show a straight line. The intersection of this with the ordinate gives $4\,B_v''$, the inclination $8\,D_v''$. To obtain the best line through the dots we used the "centre of gravity" method. This involves dividing the points into two groups each containing the same number (every average combination difference is given a weight in relation to the number of values forming it) and the centre of gravity is taken for these two groups. The two points obtained in this way give the line.

The upper levels are strongly disturbed and for this reason $\Delta^2 F'(J)/(J + \frac{1}{2})$ against $(J + \frac{1}{2})^2$ does not give straight lines. For the levels $v' = 1, 2, 3$ and

Table 4

Combination differences $\Delta^2 F''(J)$ for the lower state $v'' = 0$, obtained from the 0,0, 1,0, 2,0 and 3,0 bands

J	$R(J-1) - P(J+1)$					J	$R(J-1) - P(J+1)$				
	0,0	1,0	2,0	3,0	Mean-value		0,0	1,0	2,0	3,0	Mean-value
14	19.52	19.53			19.53	48	65.11	65.04	65.05	65.04	65.06
15	20.87	20.85	20.89	20.93	20.89	49	66.35	66.36	66.33	66.37	66.35
16	22.24	22.21	22.21	22.22	22.22	50	67.69	67.61	67.65	67.71	67.67
17	23.57	23.53	23.56	23.57	23.56	51	68.98	69.13	69.01	68.98	69.03
18	24.89	24.90	24.88	24.92	24.90	52	70.32	70.35	70.34	70.34	70.34
19	26.29	26.22	26.27	26.23	26.25	53	71.63	71.65	71.64	71.62	71.64
20	27.63	27.59	27.60	27.60	27.61	54	72.95	72.99	72.94	72.96	72.96
21	28.92	28.92	28.95	28.92	28.93	55	74.27	74.26	74.23	74.27	74.26
22	30.30	30.26	30.26	30.38	30.30	56	75.57	75.59	75.66	75.60	75.61
23	31.61	31.64	31.61	31.66	31.63	57	76.87	76.92	76.95	76.99	76.93
24	32.97	32.95	32.96	33.02	32.98	58	78.25	78.26	78.25	78.24	78.25
25	34.33	34.31	34.33	34.37	34.34	59	79.58	79.54	79.57	79.53	79.56
26	35.78	35.64	35.69	35.70	35.70	60	80.88	80.85	80.86	80.85	80.86
27	37.01	37.01	37.00	36.97	37.00	61	82.22	82.16	82.18	82.15	82.18
28	38.34	38.32	38.33	38.30	38.32	62	83.49	83.47	83.49	83.61	83.52
29	39.66	39.67	39.68	39.69	39.68	63	84.83	84.79	84.77	84.74	84.78
30	40.98	41.00	41.03	41.06	41.02	64	86.11	86.16	86.11	86.01	86.10
31	42.34	42.35	42.37	42.37	42.36	65	87.46	87.53	87.43	87.41	87.46
32	43.68	43.71	43.69	43.65	43.68	66	88.79	88.75	88.65	88.76	88.74
33	45.04	45.01	45.01	45.05	45.03	67	90.07	90.12	90.05	90.00	90.06
34	46.34	46.37	46.37	46.40	46.37	68	91.39	91.34	91.36	91.33	91.36
35	47.71	47.66	47.70	47.73	47.70	69	92.67	92.71	92.68	92.73	92.70
36	49.02	48.84	49.03	49.08	48.99	70	93.99	93.97	93.99	94.00	93.99
37	50.33	50.40	50.39	50.40	50.38	71	95.32	95.28	95.31	95.28	95.30
38	51.70	51.76	51.68	51.78	51.73	72	96.58	96.63	96.63	96.68	96.63
39	52.99	53.09	53.04	53.04	53.04	73	97.88	97.84	97.88	97.91	97.88
40	54.35	54.36	54.38	54.37	54.37	74	99.11	99.17	99.19	99.19	99.17
41	55.71	55.70	55.75	55.78	55.74	75	100.49	100.50	100.50		100.50
42	57.03	57.00	57.03	57.09	57.04	76	101.96	101.77	101.79		101.84
43	58.39	58.33	58.38	58.37	58.37	77	103.11	103.02	103.09		103.07
44	59.70	59.74	59.70	59.72	59.72	78	104.27	104.36	104.38		104.34
45	61.03	61.03	61.06	61.07	61.05	79	105.69	105.61	105.65		105.65
46	62.41	62.36	62.36	62.35	62.37	80		106.98	106.98		106.98
47	63.72	63.66	63.71	63.72	63.70	81		108.12	108.26		108.19

4 it is, however, possible to determine the influence of the perturbations and draw rather satisfactory straight lines. For the level $v' = 0$, it is more difficult to decide the position of the line.

The following constants are derived:

$B'_4 = 0.2996$ cm^{-1}; $D'_4 = 0.33 \cdot 10^{-6}$ cm^{-1};
$B'_3 = 0.3008$ $D'_3 = 0.34$
$B'_2 = 0.3021$ $D'_2 = 0.30$
$B'_1 = 0.3029$ $D'_1 = 0.31$ $B''_1 = 0.3347_4$; $D''_1 = 0.37_8 \cdot 10^{-8}$
$B'_0 = 0.303$ $D'_0 = 0.3$ $B''_0 = 0.3367_8$; $D''_0 = 0.35_4$

Table 5

Combination differences $\Delta^2 F''(J)$ for the lower state $v'' = 1$, obtained from the 0,1, 3,1 and 4,1 bands

J	$R(J-1)-P(J+1)$				J	$R(J-1)-P(J+1)$			
	0,1	3,1	4,1	Mean-value		0,1	3,1	4,1	Mean-value
14	19.37	19.43	19.41	19.40	46	61.94	61.96	61.97	61.96
15	20.75	20.81	20.73	20.76	47	63.22	63.27	63.26	63.25
16	22.10	22.17	22.07	22.11	48	64.65	64.64	64.62	64.64
17	23.36	23.35	23.38	23.36	49	65.91	65.93	65.98	65.94
18	24.83	24.75	24.65	24.74	50	67.24	67.21	67.24	67.23
19	26.15	26.22	26.05	26.14	51	68.56	68.56	68.52	68.55
20	27.28	27.39	27.46	27.38	52	69.86	69.85	69.88	69.86
21	28.76	28.76	28.75	28.76	53	71.22	71.14	71.17	71.18
22	30.13	30.20	30.15	30.16	54	72.52	72.48	72.51	72.50
23	31.43	31.48	31.41	31.44	55	73.84	73.75	73.82	73.80
24	32.75	32.74	32.76	32.75	56	75.16	75.07	75.14	75.12
25	34.18	34.06	34.09	34.11	57	76.48	76.55	76.40	76.48
26	35.43	35.37	35.39	35.40	58	77.79	77.73	77.61	77.71
27	36.77	36.83	36.77	36.79	59	79.09	78.98	78.96	79.01
28	38.10	38.06	38.05	38.07	60	80.44	80.40	80.32	80.39
29	39.43	39.39	39.34	39.39	61	81.67	81.63	81.62	81.64
30	40.73	40.74	40.75	40.74	62	83.04	82.94	82.96	82.98
31	42.07	42.08	42.10	42.08	63	84.20	84.17		84.19
32	43.35	43.42	43.27	43.35	64	85.54	85.57		85.56
33	44.81	44.73	44.83	44.79	65	86.73	86.87		86.80
34	46.11	46.07	46.10	46.09	66	88.18	88.16		88.17
35	47.49	47.42	47.39	47.43	67	89.37	89.47		89.42
36	48.66	48.69	48.72	48.69	68	90.72	90.77		90.75
37	50.04	50.13	50.10	50.09	69	92.05	92.03		92.04
38	51.31	51.42	51.39	51.37	70	93.36	93.34		93.35
39	52.53	52.67	52.57	52.59	71	94.63	94.66		94.65
40	54.01	54.01	54.06	54.03	72	95.92	95.94		95.93
41	55.30	55.37	55.34	55.34	73	97.14	97.38		97.26
42	56.53	56.64	56.72	56.63	74	98.36	98.62		98.49
43	57.95	57.98	57.98	57.97	75	99.87	99.81		99.84
44	59.37	59.31	59.30	59.33	76	101.10	101.10		101.10
45	60.63	60.65	60.64	60.64					

The constants can be collected into the equations:

$$B_v' = 0.3047_1 - 0.0011_2\,(v + \tfrac{1}{2})$$
$$B_v'' = 0.3377_9 - 0.0020_4\,(v + \tfrac{1}{2})$$
$$D_v'' = [0.34_2 + 0.02_4\,(v + \tfrac{1}{2})] \cdot 10^{-6}$$

(The D_v'-values vary rather irregularly and we do not, therefore, give an equation for them.)

The internuclear distances for the two states are:

$$r_e' = 2.02_7 \cdot 10^{-8}\ \text{cm} \qquad r_e'' = 1.92_3$$

According to Kratzer the D_e-values are:

$$D_e' = 0.291 \cdot 10^{-6}\ \text{cm}^{-1} \qquad D_e'' = 0.361 \cdot 10^{-6}$$

Vibrational analysis

The band-origins are determined for the 2,0, 1,0, 0,0 and 0,1 bands from the relation

$$R(J-1) + P(J) \simeq 2\nu_0 + (B' - B'')J^2.$$

$R(J-1) + P(J)$ are plotted against J^2. $2\nu_0$ is obtained from the intersection with the ordinate. For the other bands no straight lines were obtained as a result of the perturbations. The band-origins are given in Table 6. The calculated positions of the "unperturbed" origins of the 4,1, 3,0 and 3,1 bands are given in brackets. The vibrational constants of the upper state are derived from the known band-origins

$$\omega_e' \simeq 624\,(623.95),\quad x_e'\,\omega_e' \simeq 2\,(2.12).$$

The vibrational constants for the lower level cannot be derived from the band-origins. Approximate values can, however, be determined with the aid of the head-measurements in Table 1. We get

$$\omega_e'' = 653.4_9 \qquad x_e''\,\omega_e'' = 4.0_0.$$

The agreement with the values derived by MAHANTI for the lower level of the blue bands is good. MAHANTI obtained $\omega_e'' = 653.47$ and $x_e''\,\omega_e'' = 4.02$ cm^{-1}.

The heads of the bands emanating from $v' = 3$ are displaced about 13 cm^{-1}, the ones from $v' = 4$ about 4 cm^{-1}.

Table 6

Band-origins in cm^{-1}. Those in brackets are the unperturbed positions.

4		(12676.24)		
3	(12714.83)	(12069.25)		
2	12103.60 615.47			
1	11488.13 619.71			
0	10868.82 645.58	10222.84		
v' ↑ / v'' →	0	1	2	3

Perturbations

The upper vibrational levels show a lot of perturbations. In Fig. 3 the term values of the upper levels are drawn as functions of $J(J+1)$ $[T_v(J) = \text{const.} + G(v) + BJ(J+1) - DJ^2(J+1)^2$. The continous lines indicate the observed

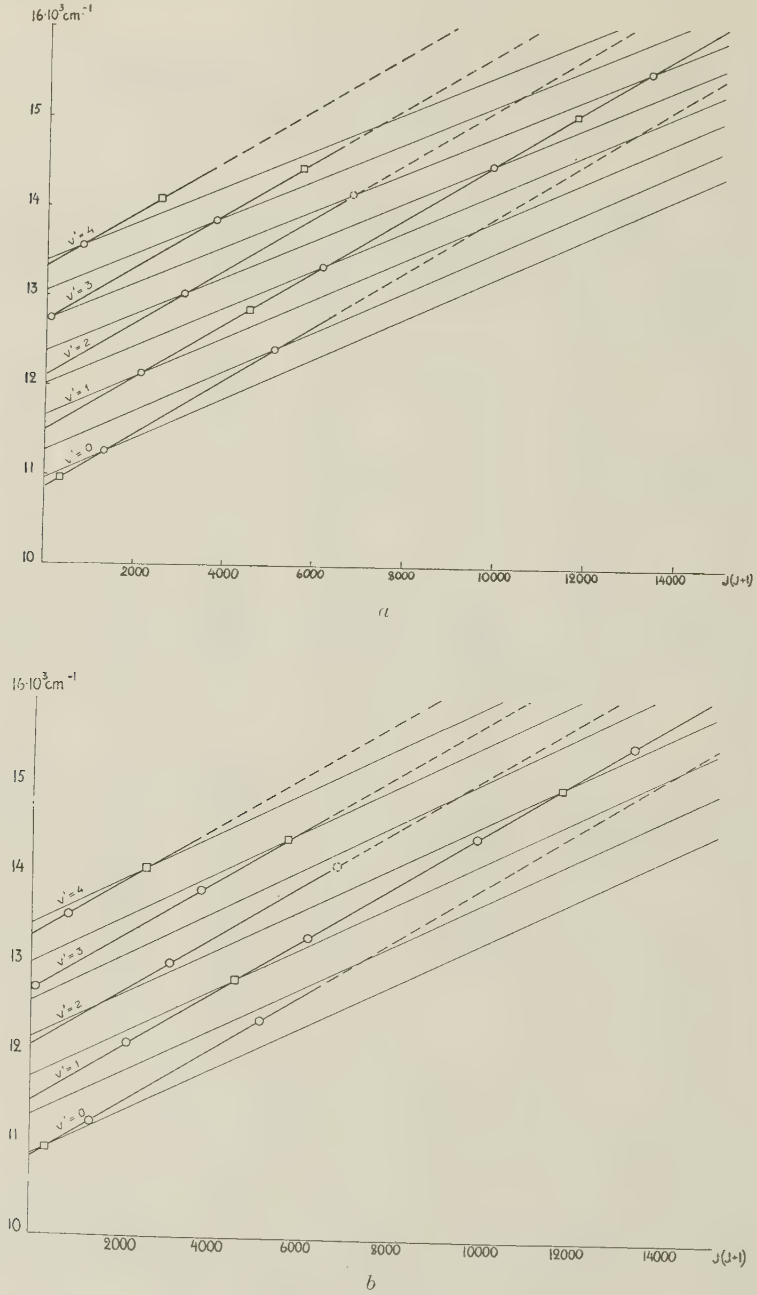
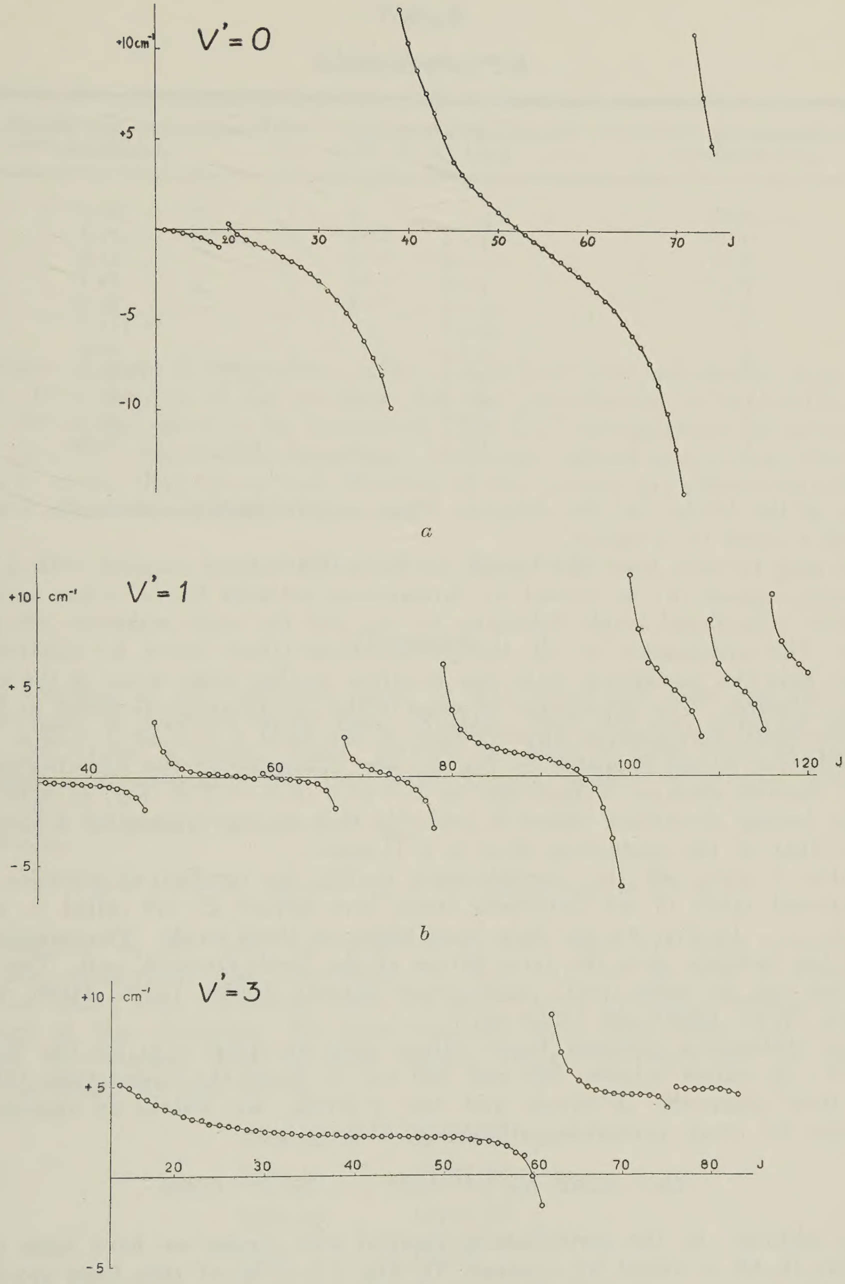


Fig. 3. Term values of Σ^* plotted against $J(J+1)$. Σ^*: analysed parts — continous, thick lines; extrapolated parts — broken, thick lines. The perturbing states: continous thin lines. Circles indicate $P\,\Sigma^*$-perturbations, squares $Q\,\Sigma^*$-perturbations. The dotted circle in $v' = 2$ marks an observed but not completely analysed perturbation.



a

b

c

Fig. 4. The appearance of the perturbations in the levels $v' = 0,1$ and 3. At higher J-values the dots have an ascending tendency. This may be the result of lasting deviations and of the existence of higher rotational constants, $F, H, \ldots$. At $J = 58.5$ in $v' = 1$ a very small perturbation appears.

Table 7

$P\Sigma^x$-perturbations

Vibrational level in Σ^x	Vibrational perturbing level (P)	J-value where the perturbation culminates
$v' = 0$	p	38.5
0	$p+1$	71.5
1	$p+2$	46.5
1	$p+3$	78.5
1	$p+4$	99.5
1	$p+5$	115.5
2	$p+4$	55.5
2	$p+5$	>83
3	$p+5$	<13
3	$p+6$	61.5
4	$p+7$	28.5

parts of the levels. At the J-values where a perturbation culminates we have placed a circle or a square.

As may be seen from the figure, all the perturbations marked with a circle certainly appear to be caused by interactions between the Σ^*-state and consecutive vibrational levels belonging to one and the same unknown electronic state. The appearance of all the perturbations (those noted by squares too) shows that the perturbing state has B-values smaller than those of the known upper Σ-levels. The appearance of some of the perturbations is shown in Fig. 4. A very small perturbation appears here in the level $v' = 1$ at $J = 58.5$. This perturbation is not indicated in Fig. 3. The character of the perturbations (a very marked example is that one at $J = 61.5$ in $v = 3$ in Fig. 4) with distinctly lasting deviations makes it probable that we have so-called Λ-perturbations, that is, the perturbing level is a Π-state.

Table 7 gives all the perturbations in Fig. 3 a marked with circles. The vibrational levels of the disturbing state, here termed P, are called p, $p + 1$, $p + 2$, ... In Fig. 3 a the thin lines represent these levels. The intersections with the ordinate gave the term values of the levels above $v'' = 0$. The intersections are in order (only approximate values): 10960, 11320, 11680, 12030, 12380, 12710, 13050 and 13390 cm^{-1}.

The differences between these values give us $\Delta G(v + \frac{1}{2})$ for the P-state. $\Delta G(v + \frac{1}{2})$ varies between 360 and 330 cm^{-1}. From the intersections between the lines from the Σ^*-levels and the P-levels, we obtain an approximate B-value for every perturbing vibrational P-level, i. e.

$$B_p \approx 0.222,\ B_{p+1} \approx 0.220\ .\ .\ .,\ B_{p+7} \approx 0.209.$$

In addition to the perturbations marked with circles we have some others — five in all — noted by squares. In Fig. 3 b a set of thin lines are drawn indicating another perturbing electronic state here termed Q causing these perturbations in the upper Σ-state. One of these levels requires a perturbation at about $J = 39$ in the Σ-level $v' = 2$, but in the 2,0 band we have not found any perturbation there. A characteristic feature of all these $Q\,\Sigma^*$-perturbations

Table 8

$Q\Sigma^x$-perturbations

Vibrational level in Σ^x	Vibrational perturbing level (q)	J-value where the perturbation culminates
$v'=0$	q	19.5
1	$q+2$	67.5
1	$q+3$	108.5
3	$q+5$	75.5
4	$q+6$	50.5

(the upper Σ-state is everywhere called Σ^*) is that they are smaller than the others. It is not out of the question that the perturbation in the level $v' = 2$ at $J \sim 39$ is too small to be discovered. The $Q\Sigma^*$-perturbations are given in Table 8. The vibrational disturbing levels are termed $q, q + 1, q + 2, \ldots$. Fig. 3 b shows that the ω and B-values of the Q-state are greater than those of the P-state. Approximate values are

$$\omega_q = 430 \ \text{cm}^{-1}; \qquad B_q = 0.245.$$

Discussion

The analysis of the infra-red bands of SrO shows that they and the blue system have a common lower state. Further, there are two unknown states below the upper Σ^*-state, which perturb it. It is of little value to discuss the dissociation energies for the three known states. With the formula $D = \frac{\omega_e^2}{4\,x_e\,\omega_e}$ we obtain, however,

$$D_\Sigma = 3.3 \ \text{e. v.}, \ (D_{\Sigma^*} = 5.7 \ \text{e. v.}), \ D_{(\text{upper blue})} = 3.3 \ \text{e. v.}$$

In addition to the blue and infra-red systems there are other systems in SrO. The ultra-violet one discovered by MAHANTI has no level in common with the other two. Further, there are surely more systems situated in the red part of the spectrum. We have measured some band-heads that do not fit into our system. The following appear rather distinctly on the plates (given in Ångström and in cm^{-1})

7208.02 Å	13869.62 cm^{-1}
7264.46	13761.86
7285.96	13721.25
7436	13444
7489.72	13347.96

It is of course a very delicate question to decide whether the lower state of the infra-red system is the ground state of the molecule or not. If, how-

Table 9

Some band-constands for BeO, MgO, SrO and BaO

Molecule	Probable ground state	Dissociation energy in e. v.	ω_e in cm^{-1}	B_e in cm^{-1}	r_e in Å
BeO	$^1\Sigma$	5.9	1487	1.6510	1.33
MgO	$^1\Sigma$	3.7	785	0.5743	1.75
SrO	$^1\Sigma$	3.3	653	0.3378	1.92
BaO	$^1\Sigma$	6.8	670	0.3123	1.94

ever, we make such an assumption we can compare SrO with the other eart alkaline oxide. Table 9 gives some data for BeO, MgO, SrO and BaO. (8, 9, 10) The values for CaO are very uncertain and for this reason they are omitte from the table above.

As it is very likely that the blue system and the infra-red one treated her have the same lower state, it would be of great interest to analyse the blu system. In a future investigation we will return to this.

We wish to express our thanks to Professor E. HULTHÉN for his keen interes in the work.

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